Uploading C:\Program Files\Stnexp\Queries\10722858.str

chain nodes :

7 8 9 10 23 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16 17 18 19 20 21 22

chain bonds :

1-26 1-27 2-28 3-9 4-7 5-24 5-25 6-23 7-8 9-10 10-16 21-29 28-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22

18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 1-6 2-3 2-28 3-4 3-9 4-5 4-7 5-6 6-23

exact bonds :

1-26 1-27 5-24 5-25 7-8 9-10 10-16 21-29 28-29

normalized bonds :

11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

Match level :

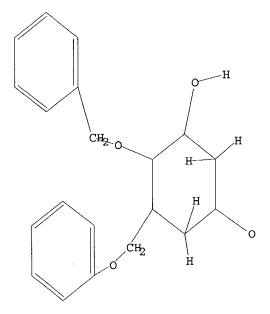
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 07:28:18 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2988 TO ITERATE

33.5% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

56482 TO 63038

PROJECTED ANSWERS:

0 TO

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 07:28:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 60313 TO ITERATE

100.0% PROCESSED 60313 ITERATIONS

0 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10722858.str

chain nodes :

7 8 9 10 23 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16 17 18 19 20 21 22

chain bonds :

1-26 1-27 2-28 3-9 4-7 5-24 5-25 6-23 7-8 9-10 10-16 21-29 28-29

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 11-12 \quad 11-16 \quad 12-13 \quad 13-14 \quad 14-15 \quad 15-16 \quad 17-18 \quad 17-22$

18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 1-6 2-3 2-28 3-4 3-9 4-5 4-7 5-6 6-23

exact bonds :

1-26 1-27 5-24 5-25 7-8 9-10 10-16 21-29 28-29

normalized bonds :

11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

20:Atom 21:Atom

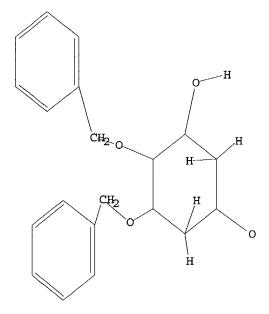
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 07:29:50 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 6358 TO ITERATE

15.7% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

122381 TO 131939

PROJECTED ANSWERS:

0 TO 0

L5

0 SEA SSS SAM L4

=> s 14 full

FULL SEARCH INITIATED 07:29:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 127772 TO ITERATE

100.0% PROCESSED 127772 ITERATIONS SEARCH TIME: 00.00.02

4 ANSWERS

L6

4 SEA SSS FUL L4

=> d scan

L6 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Cyclohexanol, 2,3,5-tris(phenylmethoxy)-, $(1\alpha,2\beta,3\alpha,5.bet$

a.)- (9CI)

MF C27 H30 O4

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L6 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Cyclohexanol, 2-[(4-methoxyphenyl)methoxy]-3,5-bis(phenylmethoxy)-,

(1R,2R,3R,5R)- (9CI)

MF C28 H32 O5

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Cyclohexanol, 5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,3bis(phenylmethoxy)-, (1R,2R,3R,5R)- (9CI)

MF C26 H38 O4 Si

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Cyclohexanol, 5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,3-

bis(phenylmethoxy)-, (1R,2R,3R,5S)- (9CI)

MF C26 H38 O4 Si

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 311.68 312.79

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 07:30:14 ON 21 APR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Apr 2004 VOL 140 ISS 17 FILE LAST UPDATED: 20 Apr 2004 (20040420/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16

L7 4 L6

=> d ibib abs hitstr 1-4

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:220342 CAPLUS

DOCUMENT NUMBER: 1

140:271144

TITLE: Preparation of cyclitols as serine/threonine kinase

Akt inhibitors

INVENTOR(S): Kozikowski, Alan P.; Dennis, Phillip; Sun, Haiying;

Brognard, John

PATENT ASSIGNEE(S): Georgetown University, USA; United States Dept. of

Health and Human Services

SOURCE:

PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE PATENT NO. KIND DATE _ _ _ _ WO 2004022569 **A1** 20040318 WO 2003-US27607 20030903 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2002-407239P P 20020903

PRIORITY APPLN. INFO.:

GI

$$OH$$
 $O-CH_2$
 $O-CH_2$
 $O-CH_2$
 $O-CH_2$
 $O-CH_2$
 $O-CH_2$
 $O-CH_2$
 $O-CH_2$

Cyclitols I, wherein X and Y are independently selected from the group consisting of O, CF2, CH2, and CHF; A is independently P(O)OH, CH2OOH, and CH(COOH)2; R2 is H, OH, isosteres of OH, C1-C25 alkyloxy, C6-C10 aryloxy, C3-C8 cycloalkyloxy, C3-C8 cycloalkyl C1-C6 alkoxy, C2-C22 alkenyloxy, C3-C8 cycloalkenyloxy, C7-C32 aralkyloxy, C7-C32 alkylaryloxy, C9-C32 aralkenyloxy, and C9-C32 alkenylaryloxy; R3-R6 are independently H, OH, isosteres of OH; and R1 and R7 are independently selected from the group consisting of C1-C25 alkyl, C6-C10 aryl, C3-C8 cycloalkyl, C2-C22 alkenyl, C3-C8 cycloalkenyl, C7-C32 aralkyl, C7-C32 alkylaryl, C9-C32 aralkenyl, and C9-C32 alkenylaryl; with the proviso that (i) when X is O, Y is O or CH2, and R3 is H, at least one of R2 and R4-R6 is not OH; (ii) when A is CH2COOH or CH(COOH)2, X and Y cannot be simultaneously O; and (iii) all of R2-R6 are not simultaneously H, were prepared as serine/threonine kinase Akt inhibitors. The inhibitors can be in the form of a salt also inhibitors of the serine/threonine kinase Akt, pharmaceutical compns. comprising such inhibitors, and a method of preventing or treating a disease or condition in an animal by the use of such inhibitors. Thus, cyclitol II was prepared

and tested as inhibitor of the serine/threonine kinase Akt for preventing or treating a disease or condition in an animal (no data). He cancer is breast cancer, lung cancer, ovarian cancer, uterine cancer, brain cancer, sarcoma, melanoma, leukemia, lymphoma, colorectal cancer, prostate cancer, or liver cancer. The rheumatol. disease is rheumatoid arthritis or osteoarthritis. The pulmonary disease is chronic obstructive pulmonary disease (COPD).

IT 671193-11-6P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of cyclitols as serine threonine kinase akt inhibitors)

RN 671193-11-6 CAPLUS

CN Cyclohexanol, 2-[(4-methoxyphenyl)methoxy]-3,5-bis(phenylmethoxy)-, (1R,2R,3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:282113 CAPLUS

DOCUMENT NUMBER:

138:287899

TITLE:

Synthesis of A-ring synthon glycoside phosphine oxide

of $19-\text{nor}-1\alpha$, 25-dihydroxyvitamin D3 from

(D) -glucose

INVENTOR(S):

Deluca, Hector F.; Shimizu, Masato; Yamada, Sachiko

Wisconsin Alumni Research Foundation, USA

PATENT ASSIGNEE(S): SOURCE:

U.S. Pat. Appl. Publ., 17 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

GΙ

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003069212	A1	20030410	US 2002-205453	20020725
US 6683219	B2	20040127		
JP 2003176250	A2	20030624	JP 2002-220721	20020730
PRIORITY APPLN. INFO.	:	US	2001-308716P P	20010730
		US	2002-205453 A	20020725
OTHER SOURCE(S):	MA	RPAT 138:287899		

R¹O OR³ CH₂ POPh₂ I

The present invention provides a method for the synthesis of an A-ring synthon phosphine oxide I, wherein R1-R3 are independently OH protecting group, used in the preparation of 19-nor vitamin D compds., and to novel synthetic intermediates formed during the synthesis. The new method preps. the phosphine oxide from (D)-glucose. Thus, I (R1 = TMS, R2 = R3 = TBS) was prepared from glucose. Some of these compds. exhibit an interesting separation of activities in cell differentiation and calcium regulation. This difference in activity may be useful in the treatment of a variety of diseases (no data). Thus, these compds. are potentially useful as therapeutic agents for the treatment of malignancies, or the treatment of various skin disorders (no data).

IT 506423-07-0P 506423-08-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of A-ring synthon glycoside phosphine oxide of $19-nor-1\alpha, 25$ -dihydroxyvitamin D3 from (D)-glucose)

RN 506423-07-0 CAPLUS

CN Cyclohexanol, 5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,3-bis(phenylmethoxy)-, (1R,2R,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 506423-08-1 CAPLUS

CN Cyclohexanol, 5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,3-bis(phenylmethoxy)-, (1R,2R,3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:162656 CAPLUS

DOCUMENT NUMBER:

139:53208

TITLE:

Novel synthesis of 2-Substituted 19-norvitamin D A-ring phosphine oxide from D-glucose as a building

block

AUTHOR(S):

Shimizu, Masato; Iwasaki, Yukiko; Shibamoto,

CORPORATE SOURCE:

Yoshinori; Sato, Miki; DeLuca, H. F.; Yamada, Sachiko Institute of Biomaterials and Bioengineering, Tokyo

Medical and Dental University, Chiyoda-ku, Tokyo,

101-0062, Japan

 ${\tt SOURCE:}$

Bioorganic & Medicinal Chemistry Letters (2003),

13(5), 809-812

CODEN: BMCLE8; ISSN: 0960-894X

Elsevier Science Ltd.

PUBLISHER: DOCUMENT TYPE:

Journal English

I

LANGUAGE: OTHER SOURCE(S):

CASREACT 139:53208

GT

19-Norvitamin D A-ring phosphine oxide I was synthesized by a new sequence AB mode starting from D-glucose as a chiral template. Transformation of the pyranoside ring into I was achieved by the Pd-catalyzed Ferrier rearrangement. I was obtained in an 18% overall yield by this novel cost-effective method.

506423-07-0P IT

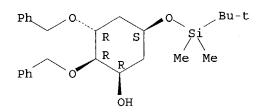
> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-substituted 19-norvitamin D A-ring building block starting from D-glucose)

506423-07-0 CAPLUS RN

Cyclohexanol, 5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,3-CN bis (phenylmethoxy) -, (1R, 2R, 3R, 5S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2004 ACS on STN L7 ANSWER 4 OF 4

ACCESSION NUMBER:

1991:492747 CAPLUS

DOCUMENT NUMBER:

115:92747

TITLE:

Design and synthesis of 6α-substituted

 2β , 4α -dihydroxy- 1β -

phosphoryloxycyclohexanes, potent inhibitors of

inositol monophosphatase

AUTHOR (S):

Baker, Raymond; Carrick, Carmel; Leeson, Paul D.;

CORPORATE SOURCE:

Lennon, Ian C.; Liverton, Nigel J.

Neurosci. Res. Cent., Merck Sharp and Dohme Res. Lab.,

SOURCE:

Harlow/Essex, CM20 2QR, UK

Journal of the Chemical Society, Chemical Communications (1991), (5), 298-300

CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE:

Journal

LANGUAGE: English CASREACT 115:92747 OTHER SOURCE(S): Mol. superimposition studies have led to the design and synthesis of 2β , 4α -dihydroxy- 6α -[5-(2-hydroxyphenyl) pentyloxy]- 1β phosphoryloxycyclohexane, a potent inhibitor of inositol monophosphatase. IT 135182-51-3P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 135182-51-3 CAPLUS RNCyclohexanol, 2,3,5-tris(phenylmethoxy)-, $(1\alpha,2\beta,3\alpha,5.bet$ CN a.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

=> s protecting group (4w) benzyl 48374 PROTECTING 1370895 GROUP 892601 GROUPS 1919345 GROUP (GROUP OR GROUPS) 13629 PROTECTING GROUP (PROTECTING (W) GROUP) 160018 BENZYL 45 BENZYLS 160033 BENZYL (BENZYL OR BENZYLS) 73 PROTECTING GROUP (4W) BENZYL L8=> s 18 and (alcohol or hydroxy) 211860 ALCOHOL 145717 ALCOHOLS 330956 ALCOHOL (ALCOHOL OR ALCOHOLS) 534265 ALC 177960 ALCS 625279 ALC (ALC OR ALCS) 742444 ALCOHOL (ALCOHOL OR ALC) 409582 HYDROXY 9 HYDROXIES 409591 HYDROXY (HYDROXY OR HYDROXIES) L9 20 L8 AND (ALCOHOL OR HYDROXY)

=> d ti 1-20

L9 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

TI Highly efficient and convenient deprotection of methoxymethyl ethers and esters using bismuth triflate in an aqueous medium

- L9 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI New penam derivative and method of preparation thereof using indium and zinc
- L9 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of sulfonyl aryl or heteroaryl hydroxamic acid compounds as inhibitors of matrix metalloproteinase
- L9 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Mild and selective sodium azide mediated cleavage of p-nitrobenzoic esters
- L9 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Catalytic, Highly Enantioselective Friedel-Crafts Reactions of Aromatic and Heteroaromatic Compounds to Trifluoropyruvate. A Simple Approach for the Formation of Optically Active Aromatic and Heteroaromatic Hydroxy Trifluoromethyl Esters
- L9 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Samarium(0) and 1,1'-Dioctyl-4,4'-Bipyridinium Dibromide: A Novel Electron-Transfer System for the Chemoselective Reduction of Aromatic Nitro Groups
- L9 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI A mild and selective cleavage of trityl ethers by carbon tetrabromide-methanol
- L9 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of $\alpha\text{-amino-}\beta\text{-sulfonyl}$ hydroxamic acid compounds as matrix metalloprotease inhibitors
- L9 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI A novel approach towards intermolecular stabilization of para-quinone methides. First complexation of the elusive, simplest quinone methide, 4-methylene-2,5-cyclohexadien-1-one
- L9 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI On the selective deprotection of trityl ethers
- L9 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of carbapenem intermediates
- L9 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of C-2' hydroxyl-benzyl protected, N-carbamate protected (2R,3S)-3-phenylisoserine for use as intermediates for the synthesis of paclitaxel
- L9 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Lewis acid-catalyzed deprotection of para-methoxybenzyl ether
- L9 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of 2-(2-azetidinon-N-yl)-2- and 3-butenoic acid derivatives and their use in the cephalosporin synthesis
- L9 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Trypsin-like protease-inhibiting peptide derivatives, their synthesis and therapeutic use
- L9 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Processes for the synthesis of diprotected R(R*,S*)-3,5-dihydroxy-6-oxohexanoate esters as intermediates for antihypercholesterolemics
- L9 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Pentapeptides as immunoregulators

- ANSWER 18 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN L9
- Hard acid and soft nucleophile system. New efficient method for removal TIof benzyl protecting group
- ANSWER 19 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN Ь9
- ΤI Alkyl 3,5-dihydroxy-4-methoxybenzoates and derivatives
- ANSWER 20 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN L9
- A new synthetic route to substituted mercaptoethylamines. Hydroxyl ΤI displacement by thiols

=> d ibib abs hitstr 12

ANSWER 12 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:719682 CAPLUS

DOCUMENT NUMBER:

127:346544

TITLE:

Preparation of C-2' hydroxyl-benzyl protected,

N-carbamate protected (2R,3S)-3-phenylisoserine for use as intermediates for the synthesis of paclitaxel

INVENTOR(S):

Sisti, Nicholas J.; Swindell, Charles S.; Chander, Madhavi C.

PATENT ASSIGNEE(S):

SOURCE:

Napro Biotherapeutics, Inc., USA; Bryn Mawr College U.S., 9 pp., Cont.-in-part of U.S. Ser. No. 357,507.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	rent :													DATE				
US	5684	 175		A		1997	1104		US	3 19	 95-4	 8308:	 1	1995	0607			
EP	1260	507		A	1	2002	1127		E	20	02-1	4256		1994	0204			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	IE
US	5770	745		Α		1998	0623		US	3 19	94-3	5750	7	1994	1215			
US	5939	566		Α		1999	0817		US	3 19	95-4	8308	3	1995	0607			
CA	2222	421		\mathbf{A}	A	1996	1219		C	A 19	96-2	2224:	21	1996	0607			
	9640																	
	W:	ΑL,	AM,	ΑT,	ΑU,	BB,	BG,	BR,	CA,	CN,	CZ,	EE,	FΙ,	GE,	HU,	IL,	IS,	
		JP,	KG,	ΚP,	KR,	LK,	LR,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MX,	NO,	NZ,	
		PL,	RO,	RU,	SG,	SI,	SK,	TR,	TT,	UA,	UΖ,	VN,	AM,	AZ,	BY,	KG,	KZ,	
		MD,	RU															
	. RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	
		ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	
		MR,	ΝE,	SN,	TD,	TG											-	
AU	9661	112		A	1	1996	1230		Α	J 19	96-6	1112		1996	0607			
AU	7015	09		В	2	1999	0128											
EP	8378	46		A	1	1998	0429		E	2 19	96-9	1845	4	1996	0607			
EP	8378	46		В	1	2001	1107											
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		ΙE,	FI															
JP	1151	4965		\mathbf{T}^{2}	2	1999	1221		JI	2 19	96-5	0216	2	1996	0607			
AT	2083	73		E		2001	1115		A.	Ր 19	96-9	1845	4	1996	0607			
ES	2166	448		T	3	2002								1996	0607			
	6262					2001	0717		US	3 19	98-2	0742		1998	0209			
ŲS	6072	060		Α		2000	0606		US	3 19	99-2	5332	5	1999	0219			
	6307					2001	1023		US	3 20	00-5	4732	7	2000	0411			
US	2002	0525	17	A	1	2002	0502		US	3 20	01-8	6388	9	2001	0522			
US	6509	484		B :	2	2003	0121											
RIORIT	APP	LN.	INFO	. :				•	US 19	993-	1509	5	B1	1993	0205			
								1	US 19	94-	3575	07	A2	1994	1215			
									EP 19	994 -	9079	73	Α3	1994	0204			
										3 O E	4000	0.1	70	1005				

US 1995-483081

A 19950607

A1 19950607 US 1995-483083 WO 1996-US10025 W 19960607 A3 19980209 US 1998-20742 US 1999-253325 A3 19990219

OTHER SOURCE(S): MARPAT 127:346544

Protected 3-phenylisoserines, (2R,3S)-PhCH(NHCO2R1)CH(OR2)CO2H (R1 = alkenyl, aryl, benzyl; R2 = hydrogenatable hydroxy

protecting group such as benzyl or

benzyloxymethyl), were prepared (no preparative examples given) as intermediates for the synthesis of paclitaxel.

=> d ibib abs hitstr 20

ANSWER 20 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1965:51038 CAPLUS

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 62.51038

62:8994e-f

TITLE:

A new synthetic route to substituted

mercaptoethylamines. Hydroxyl displacement by thiols Stacy, Gardner W.; Barnett, Buford F.; Strong, Philip

AUTHOR(S):

CORPORATE SOURCE:

Washington State Univ., Pullman

SOURCE:

Journal of Organic Chemistry (1965), 30(2), 592-7

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 62:51038

A catalytic displacement reaction of the hydroxyl group of ethynyl carbinols by thiols was accompanied by internal hydration of the acetylenic function, which enabled a new synthetic approach to substituted mercaptoethylamines. A β -oxo sulfide was converted into an oxime, $HOCMe2C.tplbond.CH \rightarrow PHCH2SH PhCH2SCMe2Ac \rightarrow$ $PhCH2SCMe2CMe:NOH \rightarrow HSCMe2CHMe:NOH \rightarrow HSCMe2CHMeNH2.$ The protecting group benzyl of the oxime was removed by reaction with Na in liquid NH3 to give an α -thiol oxime, which was reduced with LiAlH4 to yield a substituted mercaptoethylamine, wherein the thiol group was located on a tertiary C atom and the amino

=> d ibib abs hitstr 15-19

ANSWER 15 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:520428 CAPLUS

group on a secondary C atom, as in the schematic example shown.

DOCUMENT NUMBER:

122:285553

TITLE:

Trypsin-like protease-inhibiting peptide derivatives,

their synthesis and therapeutic use

INVENTOR(S):

Antonsson, Karl Thomas; Bylund, Ruth Elvy; Gustafsson,

Nils David; Nilsson, Nils Olov Ingemar

PATENT ASSIGNEE(S):

Astra Aktiebolag, Swed. PCT Int. Appl., 263 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.		KII	ND :	DATE			A	PPLI	CATIO	N NC	o. :	DATE			
									- -					-		
WO 9429	336		A	1	1994	1222		W	19	94 - SI	E535		1994	0602		
W:	ΑT,	AU,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	ES,	FI,	GB,	GE,
	HU,	JP,	KG,	ΚP,	KR,	ΚZ,	LK,	LU,	LV,	MD,	MG,	MN,	MW,	NL,	NO,	NZ,
	PL,	PT,	RO,	RU,	SD,	SE,	SI,	SK,	ТJ,	TT,	UA,	US,	UZ,	VN		

```
19990411
                                            IL 1994-109634
    IL 109634
                       A1
                            20020228
                                           HR 1994-940311
                                                             19940517
    HR 940311
                       В1
                                           CA 1994-2162900
                                                             19940602
    CA 2162900
                       AA
                            19941222
                                           AU 1994-69869
                                                             19940602
    AU 9469869
                       A1
                            19950103
    AU 684086
                       B2
                            19971204
                                           BR 1994-6746
                                                             19940602
    BR 9406746
                       Α
                            19960319
                                           EP 1994-918636
                                                             19940602
    EP 701568
                       Α1
                            19960320
    EP 701568
                       В1
                            20010425
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                                           CN 1994-192799
                                                             19940602
    CN 1127509
                       Α
                            19960724
    CN 1099425
                       В
                            20030122
    HU 74739
                                           HU 1995-3445
                                                             19940602
                            19970228
                       Α2
    RU 2142469
                                                             19940602
                            19991210
                                            RU 1996-101161
                       C1
                                           EP 2000-121659
                                                             19940602
    EP 1067136
                       Α1
                            20010110
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI
                       Ε
                            20010515
                                            AT 1994-918636
                                                             19940602
    AT 200783
                                            ES 1994-918636
    ES 2128277
                       T3
                            20010701
                                                             19940602
    PT 701568
                       Т
                                            PT 1994-94918636 19940602
                            20010830
    JP 3205558
                                            JP 1995-501665
                       B2
                            20010904
                                                             19940602
    PL 181968
                                           PL 1994-311819
                                                             19940602
                       B1
                            20011031
    JP 2001322974
                       A2
                            20011120
                                            JP 2001-91958
                                                             19940602
    JP 2002047264
                       A2
                            20020212
                                           JP 2001-158596
                                                             19940602
                                            CZ 1995-3020
    CZ 290104
                       B6
                            20020515
                                                             19940602
                                            SK 1995-1454
    SK 283150
                       В6
                            20030304
                                                             19940602
    LT 3768
                                           LT 1994-1947
                       В
                            19960325
                                                             19940603
                                           EE 1994-456
    EE 3264
                       В1
                            20000417
                                                             19941123
    US 5602253
                       Α
                            19970211
                                           US 1995-468046
                                                             19950606
    US 5723444
                       Α
                            19980303
                                           US 1995-470277
                                                             19950606
    US 5780631
                            19980714
                                           US 1995-465916
                                                             19950606
                       Α
    US 5783563
                            19980721
                                           US 1995-470258
                                                             19950606
                       Α
                       Α
                            19990105
                                           US 1995-484427
                                                             19950607
    US 5856307
                       Α
                            19990817
                                           US 1995-481811
                                                             19950607
    US 5939392
    NO 9504873
                       Α
                            19960201
                                           NO 1995-4873
                                                             19951130
                       Α
                                            FI 1995-5828
    FI 9505828
                            19951204
                                                             19951204
                            20010103
                                            CN 1999-124859
                                                             19991115
     CN 1278530
                       Α
                       Т3
                            20011031
                                            GR 2001-401107
                                                             20010724
    GR 3036258
PRIORITY APPLN. INFO.:
                                         SE 1993-1916
                                                          A 19930603
                                         EP 1994-918636
                                                          A3 19940602
                                         JP 1995-501665
                                                          A3 19940602
                                         JP 2001-91958
                                                          A3 19940602
                                         WO 1994-SE535
                                                          W 19940602
                                         US 1994-382036
                                                          A1 19940819
AB
     The invention relates to peptide derivs. which are competitive inhibitors
     of trypsin-like serine proteases, their synthesis, pharmaceutical compns.
     containing the compds. as active ingredients, and the use of the compds. as
     thrombin inhibitors, anticoagulants and anti-inflammatory inhibitors for
     prophylaxis and treatment of related diseases. Further described are
     novel compds., the new use of compds. and especially new structural fragments
in
     synthesis of pharmaceutical compds. Numerous peptide derivs. were prepared
    HO2CCH2-(R)-Cql-Aze-Pab [Cql = cyclohexylqlycine, Aze =
     azetidine-2-carboxylic acid, Pab = 4-aminomethyl-1-(N-
     benzyloxycarbonylamidino)benzene] was prepared by carbodiimide-mediated
     coupling of Boc-(R)-Cgl-Aze-OH with Pab-Z, removal of the Boc
```

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

TW 403731

В

20000901

TW 1994-83104085 19940505

19940512

ANSWER 16 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1990:197638 CAPLUS

-2-(o-nitrobenzenesulfonyloxy)acetate, removal of the Z protecting

group, and removal of the benzyl group by hydrogenation.

protecting group, alkylation with benzyl

DOCUMENT NUMBER:

112:197638

TITLE:

Processes for the synthesis of diprotected

R(R*,S*)-3,5-dihydroxy-6-oxohexanoate esters as

intermediates for antihypercholesterolemics

INVENTOR(S):

Chen, Kau Ming; Hardtmann, Goetz E.; Kapa, Prasad K.; Lee, George T.; Linder, Jerome; Wattanasin, Sompong

PATENT ASSIGNEE(S):

Sandoz Pharmaceuticals Corp., USA

SOURCE:

U.S., 23 pp. Cont.-in-part of U.S. Ser. No. 857,689,

abandoned.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4870199	A	19890926	US 1988-166594	19880310
PRIORITY APPLN. INFO.	:		US 1986-857689	19860430
			IIS 1987-23079	19870306

OTHER SOURCE(S):

MARPAT 112:197638

R[R*,S*]-OHCCH(OR1)CH2CH(OR2)CH2CO2R3 (I; R1, R2 = protecting group; R3 = alkyl, allyl, benzyl), useful as intermediates for HMG CoA reductase inhibitors trans-R4HC: CHCH (OH) CH2CH (OH) CH2CO2H (II) [R4 = (substituted) Ph, biphenylyl, indolyl, diphenylimidazolyl, diphenylpyrazolyl, etc.], were prepared, e.g., from S-Ph3COCH2CH(OH)CH2CO2H via (1) condensation with Mg(O2CCH2CO2R3)2, (2) stereoselective reduction of the resulting S-Ph3COCH2CH(OH)CH2COCH2CO2R3 to the corresponding R[R*,S*]-diol, (3) protection of the diol, (4) cleavage of the triphenylmethyl group, and (5) oxidation to the aldehyde. Thus, S-Ph3COCH2CH(OH)CH2CO2Me (preparation given) in THF was added to a mixture

of MeCO2CMe3 and Li diisopropylamide in THF at -62 to -60° over 25 min. The mixture was stirred at that temperature for 1 h followed by gradual warming to give 87.1% S-Ph3OCH2CH(OH)CH2COCH2CO2CMe3. The latter was reduced with Et3B and NaBH4 in MeOH/THF to give the corresponding diol with a 69:1 ratio of $R[R^*,S^*]$ to $S[R^*,R^*]$ -stereoisomers. The diol was bis-silylated with Me3CSiPh2Cl, detritylated with CF3CO2H, and oxidized with pyridinium chlorochromate to give R[R*,S*]-OHCCH(OSiPh2CMe3)CH2CH(OSiPh2CMe3)CH2CO2CMe3. Several II were prepared from I and phosphonate reagents.

ANSWER 17 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1986:573053 CAPLUS

DOCUMENT NUMBER:

105:173053

TITLE:

SOURCE:

Pentapeptides as immunoregulators

INVENTOR(S):

Koenig, Wolfgang; Geiger, Rolf; Obermeier, Rainer;

Muellner, Hubert

PATENT ASSIGNEE(S):

Hoechst A.-G., Fed. Rep. Ger.

Ger. Offen., 16 pp.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3421614	A1	19851212	DE 1984-3421614	19840609
EP 164654	A2	19851218	EP 1985-106652	19850530
EP 164654	A3	19880113		
R: AT, BE,	CH, DE	, FR, GB,	IT, LI, NL, SE	
DK 8502549	Α	19851210	DK 1985-2549	19850606
AU 8543423	A1	19851212	AU 1985-43423	19850607

AU 588237 JP 1985-122858 19850607 A2 19860107 JP 61001700 19860226 ZA 1985-4331 19850607 ZA 8504331 Α ES 1985-543973 19850607 ES 543973 A1 19860801 19870414 US 1985-742441 19850607 US 4658016 Α PRIORITY APPLN. INFO.: DE 1984-3421614 19840609 CASREACT 105:173053 OTHER SOURCE(S): H-Arg-Lys X-Val-Y [X = L- or D-glutamic acid or α -aminoadipic acid residue; Y = L- or D-Tyr, -Trp ester or amide residue, etc.], useful as immunoregulators (no data), were prepared via condensation of H-Arg(Z1)2-Lys(Z1)-X(Bzl)-Val-OH [Z1 = amino-protecting group of the benzyl type] with the appropriate tyrosine or tryptophan ester or amide and subsequent deprotection by hydrogenolysis, etc. Thus, N-ethylmorpholine and dicyclohexylcarbodiimide were added to a mixture of Z-Arg(Z2)-Lys(Z)-Glu(OBz1)-Val-OH, $H-Tyr-OBzl\cdot Tos-OH$ (Z = PhCH2O2C, Bzl = PhCH2), and 3hydroxy-4-oxo-3,4-dihydro-1,2,3-benzotriazine at 0° and the resulting mixture stirred for 2 h at 0° and then 4 h at room temperature to qive 81% Z-Arg(Z2)-Lys(Z)-Glu(OBzl)-Val-Trp-OH·AcOH.

ANSWER 18 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1979:202998 CAPLUS

DOCUMENT NUMBER:

90:202998

19890914

B2

TITLE:

Hard acid and soft nucleophile system. New efficient

method for removal of benzyl protecting group

AUTHOR(S):

Fuji, Kaoru; Ichikawa, Kohei; Node, Manabu; Fujita,

Eiichi

CORPORATE SOURCE:

Inst. Chem. Res., Kyoto Univ., Uji, Japan

SOURCE:

Journal of Organic Chemistry (1979), 44(10), 1661-4

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Aliphatic and aromatic benzyl ethers were cleaved on treatment with a hard acid.

F3B.OEt2, and a soft nucleophile, EtSH or HSCH2CH2SH, to give parent alcs. and phenols, resp. Competitive debenzylation expts. showed that the coordination of a hard acid (pulling factor) is more important than the nucleophilic attack of a soft nucleophile to the carbon atom (pushing factor) in this reaction. Thus, benzyl 2-naphthyl ether was treated with F3B.OEt2 and EtSH at room temperature for 0.8 h to give 92% 2-naphthol. Treatment of estradiol dibenzyl ether (I) with F3B.OEt2 and EtSH in CH2Cl2 at room temperature for 3 h gave 26.39% I, 11.7% estradiol 17-monobenzyl ether, 17.5% 3-monobenzyl ether, and 30.1% estradiol.

ANSWER 19 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1969:524920 CAPLUS

DOCUMENT NUMBER:

71:124920

TITLE:

Alkyl 3,5-dihydroxy-4-methoxybenzoates and derivatives

Haeusermann, Werner; Kaiser, Ado; Scheer, Marcel INVENTOR(S):

PATENT ASSIGNEE(S):

Hoffmann-La Roche, F., und Co., A.-G. Ger. Offen., 27 pp.

SOURCE:

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	TENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE	1902583	A	19690828	DE 1969-1902583	19690120
NL	6818531	Α	19690812	NL 1968-18531	19681223
US	3622610	A	19711123	US 1969-791793	19690116
BE	727979	Α	19690806	BE 1969-727979	19690206
FR	2001654	A1	19690926	FR 1969-2934	19690207

US 3766245 A 19731016 US 1971-121158 19710304 PRIORITY APPLN. INFO.: CH 1968-1972 19680209 US 1969-791793 19690116

GΙ For diagram(s), see printed CA Issue. The title compds. (I) are prepared by the selective removal of the AΒ protecting group from C-4 of an alkyl 3,4,5-tris(substituted sulfonyloxy) benzoate in liquid NH3, methylation, and substitution of the protecting groups with benzyl halides in the presence of base; or by selective protection of the OH groups at C-3 and C-5 of alkyl gallates with alkenyl ethers, preferably vinyl Et ether or dihydropyran (II), methylation at C-4, acid hydrolysis to give the 3,5-dihydroxy analog, and benzylation to give I. These compds. are intermediates in the preparation of medicinals. Thus, 60 g. of Me 3,4,5-tris(phenylsulfonyloxy)benzoate, m. 119-21°, prepared by treating Me gallate (III) with PhSO2Cl in C5H5N, is heated 14 hours at 23° with 300 ml. liquid NH3 in an autoclave, the NH3 evaporated, and the residue heated at 50° with 300 ml. MeOH and 400 ml. H2O, cooled to 10°, and the solid thus formed suspended at 50° in 200 ml. H2O. The suspension is acidified to pH 2 with 2N H2SO4, cooled, and filtered to give Me 3,5-bis(phenylsulfonyloxy)-4-hydroxybenzoate (IV), m. 157-60° (MeOH). A mixture of 30.9 g. IV in 288 ml. HCONMe2, 11.5 g. Me2SO4, and 36 g. K2CO3 is stirred at 70° 14 hrs., the insol. materials filtered off, the solvents evaporated in vacuo and the oily residue crystallized from warm 2N HOAc to give IV 4-methoxy analog (V), m. 105-7° (MeOH). V (15 g.) is stirred at reflux under Ar 24 hrs. with 300 ml. MeOH, 20 g. BzCl, and 22 g. K2CO3 to give I Me ester (VI), m. 114-16°. Similarly prepared are the following compds. (m.p. given): Me 3,4,5-tris(methylsulfonyloxy)benzoate, 159-62° (CH2Cl2-MeOH); Me 4-hydroxy-3,5-bis (methylsulfonyloxy) benzoate, 143-6° (MeOH); and Me 3,5-bis(methylsulfonyloxy)-4-methoxybenzoate, 95-8° (EtOAcEt2O). The reaction of 20 g. III with 38 g. II and 0.05 ml. POCl3 in 40 ml. tetrahydrofuran gives a solution of Me 3,5-bis(tetrahydropyranyloxy) -4-methoxybenzoate which is heated 12 hrs. at 70° under N with K2CO3 and Me2SO4 in 400 ml. HCONMe2, the solution evaporated, and the residue refluxed 1 hour with 1 q. HO2CCO2H in 100 ml. MeOH to give Me 4-O-methylgallate (VIII). To a stirred solution of VIII and K2CO3 in HCONMe2 is added PhCH2Cl and the mixture stirred 2.5 hrs. at 90-5° to give VI, m. 120-2°. Similarly prepared is Me 3,5-bis(ethoxyethoxy)-4methoxybenzoate (a dark red liquid), from which are prepared VII, m. 135-8°, and VI. Reduction of V with LiAlH4 in tetrahydrofuran gives 3,5-bis(benzyloxy)-4-methoxybenzyl alc., m. 100°, which with SOCl2 gives the chloride (IX), m. 76-8°. A solution of (EtO2C)2CHNHAc in HCONMe2 is added slowly to a vigorously stirred suspension of NaH in HCONMe2, the resulting solution added slowly to a solution of IX in HCONMe2, and after 3-5 hrs. stirring the solution acidified to give di-Et [3,5-bis(benzyloxy)-4-methoxybenzyl]acetamidomalonate, m. 104-6°. This compound is refluxed 6-7 hrs. with aqueous NaOH and the solution acidified to pH 1 to give (±)-3,5-bis(benzyloxy)-4-methoxyphenyl-N-acetylalanine, m. 146-7°. Hydrogenation with Pd/C in EtOH followed by refluxing 4-5 hrs. with 2N HCl gives (±)-(3,5-dihydroxy-4methoxyphenyl)-alanine, m. 272-5°, which contains 1.5 mole H2O of crystallization The anhydrous amino acid (X), obtained on heating in high vacuum at

100°, is very hygroscopic and has a blood pressure lowering effect.

=> file beilstein		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	62.27	375.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.62	-7.62

FILE 'BEILSTEIN' ENTERED AT 07:44:03 ON 21 APR 2004 COPYRIGHT (c) 2004 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002 FILE LAST UPDATED ON MARCH 30,2004

FILE COVERS 1771 TO 2003.

*** FILE CONTAINS 8,932,479 SUBSTANCES ***

>>> PLEASE NOTE: Reaction data and substance data are stored in separate documents and can not be searched together in one query.

Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

=> d his

(FILE 'HOME' ENTERED AT 07:25:20 ON 21 APR 2004)

FILE 'STNGUIDE' ENTERED AT 07:25:33 ON 21 APR 2004

FILE 'HOME' ENTERED AT 07:25:37 ON 21 APR 2004

FILE 'REGISTRY' ENTERED AT 07:28:05 ON 21 APR 2004
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 FULL
L4 STRUCTURE UPLOADED

L5 0 S L4

L6 4 S L4 FULL

FILE 'CAPLUS' ENTERED AT 07:30:14 ON 21 APR 2004

L7 4 S L6

73 S PROTECTING GROUP (4W) BENZYL

L9 20 S L8 AND (ALCOHOL OR HYDROXY)

FILE 'BEILSTEIN' ENTERED AT 07:44:03 ON 21 APR 2004

L8

FULL SEARCH INITIATED 07:54:41 FILE 'BEILSTEIN' FULL SCREEN SEARCH COMPLETED - 66555 TO ITERATE

50.5% PROCESSED 33580 ITERATIONS 0 ANSWERS

89.5% PROCESSED 59560 ITERATIONS 2 ANSWERS

100.0% PROCESSED 66555 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.47

L10 2 SEA SSS FUL L4

=>

=> d ide

L10 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9356951

Chemical Name (CN): 2,3-bis-benzyloxy-5-(tert-butyl-dimethyl-

silanyloxy) -cyclohexanol

Autonom Name (AUN): 2,3-bis-benzyloxy-5-(tert-butyl-dimethyl-

silanyloxy) -cyclohexanol

Molec. Formula (MF): C26 H38 O4 Si

Molecular Weight (MW): 442.67

Lawson Number (LN): 6630, 5228, 3798, 3777

File Segment (FS): Stereo compound

Compound Type (CTYPE): isocyclic Constitution ID (CONSID): 7895130 Tautomer ID (TAUTID): 8767133 Entry Date (DED): 2003/07/25 Update Date (DUPD): 2003/07/25

Field Availability:

Code	Name	Occurrence
=======		========
BRN	Beilstein Records	1

CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
========		=========
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d frxpro

L10 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9282856 Reactant BRN (.RBRN): 9355400

Reactant (.RCT): 2,3-bis-benzyloxy-5-(tert-butyl-dimethyl-

silanyloxy) -cyclohexanone

Product BRN (.PBRN): 9356951

Product (.PRO): 2,3-bis-benzyloxy-5-(tert-butyl-dimethyl-

silanyloxy) -cyclohexanol

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 9282856.1
Reaction Classification (.CL): Preparation

Yield (.YDT): 95 percent (BRN=9356951)

Reagent (.RGT): L-Selectride Solvent (.SOL): tetrahydrofuran

Reference(s):

 Shimizu, Masato; Iwasaki, Yukiko; Shibamoto, Yoshinori; Sato, Miki; DeLuca, H. F.; Yamada, Sachiko, Bioorg.Med.Chem.Lett., CODEN: BMCLE8, 13(5), <2003>, 809 - 812; BABS-6388022

=> d ide 2 frxpro

L10 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9356950

Chemical Name (CN): 2,3-bis-benzyloxy-5-(tert-butyl-dimethyl-

silanyloxy) -cyclohexanol

Autonom Name (AUN): 2,3-bis-benzyloxy-5-(tert-butyl-dimethyl-

silanyloxy) -cyclohexanol

Molec. Formula (MF): C26 H38 O4 Si

Molecular Weight (MW): 442.67

Lawson Number (LN): 6630, 5228, 3798, 3777

File Segment (FS): Stereo compound

Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	7895130
Tautomer ID (TAUTID):	8767132
Entry Date (DED):	2003/07/25
Update Date (DUPD):	2003/07/25

Field Availability:

Code	Name	Occurrence
======		
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
		
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:

RX

Reaction ID (.ID):

Reactant BRN (.RBRN):

Reactant (.RCT):

Product BRN (.PBRN):

Product (.PRO):

Product